THE SOLUTION OF THE NONLINEAR POISSON-BOLTZMANN EQUATION USING LATTICE-BOLTZMANN

SOLUCIÓN DE LA ECUACIÓN NO-LINEAL DE POISSON-BOLTZMANN USANDO EL MÉTODO DE LATTICE-BOLTZMANN

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ABSTRACT

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In this paper we present the solution of the Poisson-Boltzmann equation using the Lattice-Boltzmann method. In order to obtain the solution, we use a redefinition of tensor Π^0, which is declared as a symmetric tensor whose diagonal components are chosen as the second derivative in time of the first moment of the distribution function, and the components outside of the diagonal give account of the nonlinear terms. The results are presented in two dimensions employing the D2Q9 lattice velocity scheme. We obtain results for the scalar field and its gradient for several kinds of initial conditions.

Key words: Poisson-Boltzmann Equation, lattice-Boltzmann.

RESUMEN

En este trabajo se presentala solución de la ecuación de Poisson-Boltzmann utilizando el método de Lattice-Boltzmann. Con el fin de obtener la solución utilizamos una redefinición del tensor Π^0, el cual se declara como un tensor simétrico,cuyas componentesdiagonales se eligen como la segunda derivada en el tiempo del primer momento de la función de distribución y las componentes fuera de la diagonal dan cuenta de los términos no lineales. Losresultados se presentan en dosdimensiones empleando el esquema de rejillas de velocidades D2Q9. Se obtienen resultados para el campo escalar y su gradiente usando varios tipos de condiciones iniciales.

Palabras clave: Ecuación de Poisson-Boltzmann, lattice-Boltzmann.

1. Introduction

The study of Poisson-Boltzmann (PB) equation gives the semiconductor equilibrium energy band for heterostructures (**Lundstrom M. S., Schuelke R. J.** , 1982). Also PB it is very important in the biological sciences, because of the principal role of electrostatics interaction (**Luo G.**, et. al, 2006). The dynamics become more complex when they are mixed biomaterials with low dimensional semiconductors (**Cui Y., et. al**, 2001). On the other hand, a few analytical problems can be solved from weakly charged distributions.

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Therefore, a lot of work has been done implementing computational techniques in the solution of PB equation, e.g., a combination of a Garlerkin discretization method, the boundary element method, interface methods; a Newton-Krylov method, finite element methods, lattice-Boltzmann, etc. For a discussion of the different computational methods and their efficiency applied to the PB equation the reference (**Lu B. Z. et al.**, 2008) is suggested.

On the other hand, lattice-Boltzmann (LB) has been applied with success to many problems in Physics, and in particular, we find a previous paper (**Wang M., Wang J. and Chen S.**, 2007) on the application of LB to study effects of cavitation and roughness in micro-channels for electro-osmotic flows. Basically, the electric potential and the pressure are introduced as an external force term in the LB expansion. Unlike this approach, our work uses the redefinition of Π^0 tensor of the distribution function as a way to obtain the PB equation.

This manuscript is organized as follows. In section (2) we present the lattice Boltzmann method and the moments of the distribution. Section (3) shows deduction of the PB equation using the definition of the Π^0 tensor. Section (4) presents the equilibrium distribution function, based on **D2Q9** scheme that gives rise to PB equation. In section (5) we present results and in section (6) we give conclusions.

2. The lattice-Boltzmann model

This is considered a bi-dimensional model where the velocities of particles are discretized on the grid into d directions. The lattice-Boltzmann equation is:

$$f_i(\vec{x} + \vec{e}_x\delta t, t + \delta t) - f_i(\vec{x}, t) = \Omega_i(\vec{x}, t) \tag{1}$$

where f_i is the probability density function of finding the group particle i, in the spatial point $\vec{x}$ and time t and δt is the time step. Ω_i is the collision term. It is defined as:

$$\Omega_i(\vec{x}, t) = -\frac{1}{\tau}(f_i(\vec{x}, t) - f^{eq}{}_i(\vec{x}, t)) \tag{2}$$

The collision operator, Eq. (2), is expressed using the B.G.K. approximation (**Bathnagar P. L., Gross E. P. and Krook M.**, 1954), where τ is the non-dimensional relaxation time that measures the approaching rated to the statistical equilibrium. Expanding the left-hand side of Eq. (1) up to second order, in a Taylor series, and using ε as a time step unit, we have:

$$f_i(\vec{x} + \vec{e}_\alpha\varepsilon, t + \varepsilon) - f_i(\vec{x}, t) = \varepsilon\left(\frac{\partial}{\partial t} + e_x\frac{\partial}{\partial x_1} + e_y\frac{\partial}{\partial y_1}\right)f_i + \frac{\varepsilon^2}{2}\left(\frac{\partial}{\partial t} + e_x\frac{\partial}{\partial x_1} + e_y\frac{\partial}{\partial y_1}\right)^2 f_i \tag{3}$$

Assuming the spatial and temporal derivatives as:

$$\frac{\partial}{\partial x} = \mathcal{E}\frac{\partial}{\partial x_1} \tag{4}$$

$$\frac{\partial}{\partial y} = \mathcal{E}\frac{\partial}{\partial y_1} \tag{5}$$

$$\frac{\partial}{\partial t} = \mathcal{E}\frac{\partial}{\partial t_1} + \mathcal{E}^2\frac{\partial}{\partial t_2} \tag{6}$$

Expanding the distribution function f_i in a perturbative series:

$$f_i = f^0{}_i + \mathcal{E}f^1{}_i + \mathcal{E}^2 f^2{}_i \tag{7}$$

we obtain at first order in $\mathcal{E}$:

$$-\frac{1}{\tau}(\mathcal{E}f^1{}_i) = \delta t(\mathcal{E}\frac{\partial}{\partial t_1} + \mathcal{E}e_x\frac{\partial}{\partial x_1} + \mathcal{E}e_y\frac{\partial}{\partial y_1})f^0{}_i \tag{8}$$

and at second order in ε:

$$-\frac{1}{\tau}\mathcal{E}^2 f^2{}_i = \mathcal{E}^2\delta t\frac{\partial}{\partial t_2}f^0{}_i + \frac{\delta t^2}{2}\left(\mathcal{E}\frac{\partial}{\partial t_1} + e_x\mathcal{E}\frac{\partial}{\partial x_1} + \mathcal{E}e_y\frac{\partial}{\partial y_1}\right)^2 f^0{}_i + \delta t(\mathcal{E}\frac{\partial}{\partial t_1} + e_x\mathcal{E}\frac{\partial}{\partial x_1} + \mathcal{E}e_y\frac{\partial}{\partial y_1})\mathcal{E}f^1{}_i \tag{9}$$

where it is assumed that

$$f^0{}_i = f^{eq}{}_i \tag{10}$$

Inserting Eq. (8) in Eq. (9), we obtain:

$$-\frac{1}{\tau}\left(\mathcal{E}f^1{}_i + \mathcal{E}^2 f^2{}_i\right) = \left(\frac{\partial}{\partial t_1} + e_x\frac{\partial}{\partial x_1} + e_y\frac{\partial}{\partial y_1}\right)(\mathcal{E}f^0{}_i + \mathcal{E}^2 f^1{}_i\left(1 - \frac{1}{2\tau}\right)) + \mathcal{E}^2\left(\frac{\partial f^0{}_i}{\partial t_2}\right) \tag{11}$$

Replacing eq. (9) in (11), we obtain:

$$-\frac{1}{\tau}f^2{}_i = \frac{\partial f^0{}_i}{\partial t_2} + (1 - \frac{1}{2\tau})\left(\frac{\partial}{\partial t_1} + e_x\frac{\partial}{\partial x_1} + e_y\frac{\partial}{\partial y_1}\right)f^1{}_i \tag{12}$$

The moments of the distribution function are defined as:

$$\rho = \Sigma_i f^0{}_i \tag{13}$$

$$\vec{u} = \Sigma_i \vec{e}_i f^0{}_i \tag{14}$$

$$\Pi^0 = \Sigma_i \vec{e}_i \cdot \vec{e}_i f^0{}_i, \tag{15}$$

$$\Sigma_i f^k{}_i = 0,\ k > 0 \tag{16}$$

$$\Sigma_i \vec{e}_i f^k{}_i = 0,\ k > 0 \tag{17}$$

Also we assume the distribution function f_i satisfies the probability conservation condition with the equilibrium distribution ${f^{eq}}_i$ such that:

$$\sum_{i=0}^{N} {f^{eq}}_i = \sum_{i=0}^{N} {f^{0}}_i \tag{18}$$

3. The Poisson-Boltzmann equation

We do the summation about (i) in Eqs. (8) and (9), and computing (8) and (9)x($\vec{e}_\alpha$), we get:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{u} = 0 \tag{19}$$

and

$$\frac{\partial \vec{u}}{\partial t} + \nabla \cdot \Pi^0 = 0 \tag{20}$$

We assume Π^0 as a symmetric tensor given by:

$${\Pi_{\mu\nu}}^0 = \frac{\partial^2 \rho}{\partial t^2}\delta_{\mu\nu} + (1-\delta_{\mu\nu})(\rho - \kappa^2 \sinh(\rho)) \tag{21}$$

where κ^2 is a constant. Replacing Eq. (21) and (21-a) in Eq. (20), we obtain for the diagonal components of the tensors:

$$\frac{\partial \vec{u}}{\partial t} + \nabla\left(\frac{\partial^2 \rho}{\partial t^2}\right) = 0 \tag{22}$$

and the off-diagonal components are:

$$\nabla(\rho - \kappa^2 \sinh(\rho)) = 0 \tag{23}$$

and we assume it as:

$$(\rho - \kappa^2 \sinh(\rho)) = 0 \tag{24}$$

Then eq. (23)

$$\frac{\partial}{\partial t}(\vec{u} + \frac{\partial}{\partial t}\nabla(\rho)) = 0 \tag{25}$$

assuming

$$\vec{u} + \frac{\partial}{\partial t}\nabla(\rho) = 0 \tag{26}$$

Taking divergence

$$\nabla.\vec{u} + \frac{\partial}{\partial t}\nabla^2(\rho) = 0 \tag{27}$$

Using Eq. (19)

$$-\frac{\partial \rho}{\partial t} + \nabla^2(\rho) = 0 \tag{28}$$

Taking out the temporal derivative

$$\frac{\partial}{\partial t}(\rho - \nabla^2(\rho)) = 0 \tag{29}$$

assuming

$$\rho - \nabla^2(\rho) = 0 \tag{30}$$

Using eq. (24), we have the Poisson-Boltzmann equation:

$$\nabla^2 \rho = \kappa^2 \sinh(\rho) \tag{31}$$

4. The equilibrium distribution function

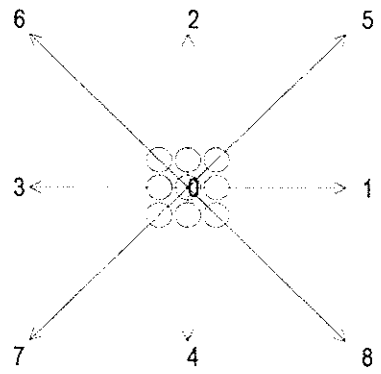

Fig.1. The lattice velocities of the **D2Q9** scheme.

We use the **D2Q9** velocity scheme shown in fig. (1), for the directions $\vec{e}_i$ and weights w_i on each cell:

$$w_i = \begin{Bmatrix} \frac{4}{9} & \rightarrow & i = 0 \\ \frac{1}{9} & \rightarrow & i = 1,2,3,4 \\ \frac{1}{36} & \rightarrow & i = 5,6,7,8 \end{Bmatrix} \tag{32}$$

Both directions $\vec{e}_i$ and weights w_i follow the next set of tensor relations:

$$\sum_i w_i \, e_{i,\alpha} = 0 \tag{33}$$

$$\sum_i w_i \, e_{i,\alpha} e_{i,\beta} = \frac{1}{3}\delta_{\alpha,\beta} \tag{34}$$

$$\sum_i w_i \, e_{i,\alpha} e_{i,\beta} e_{i,\gamma} = 0 \tag{35}$$

Also, we assume the equilibrium function

$${f^{eq}}_i = \begin{Bmatrix} w_i(A + B\vec{e}_i \cdot \vec{u}) & i > 0 \\ w_0 C & i = 0 \end{Bmatrix} \tag{36}$$

Using Equations (13-17) that define the moments of the distribution, and also the set of equations that give the tensor relations of the lattice velocity equations (27-28), we obtain:

$$A = 3\left(\frac{\partial^2\rho}{\partial t^2} - \kappa^2\rho - \kappa^2\sinh(\rho)\right) \tag{37}$$

$$B = 3 \tag{38}$$

$$C = \frac{9}{4}\rho - \frac{5}{4}\left(\frac{\partial^2\rho}{\partial t^2} - \kappa^2\rho - \kappa^2\sinh(\rho)\right) \tag{39}$$

Then, the equilibrium distribution function that satisfies the Helmholtz equation is:

$$f^{eq}{}_i = \begin{cases} 3w_i\left(\vec{e}_i\cdot\vec{u} + \left(\frac{\partial^2\rho}{\partial t^2} - \kappa^2\rho - \kappa^2\sinh(\rho)\right)\right) & i > 0 \\ w_0\left(\frac{9}{4}\rho - \frac{5}{4}\left(\frac{\partial^2\rho}{\partial t^2} - \kappa^2\rho - \kappa^2\sinh(\rho)\right)\right) & i = 0 \end{cases} \tag{40}$$

5. Analysis and Results

We use the difference discretization scheme of the second derivative, in order to apply the distribution function, as:

$$\frac{\partial^2\rho}{\partial t^2} = \frac{\rho(x,t+\delta t) - \rho(x,t) + \rho(x,t-\delta t)}{\delta t^2} \tag{41}$$

The system is initialized with the function:

$$f_i(x,y,0) = A_1 sin(D(x+2)^2 + D(y+2)^2) \tag{42}$$

and

$$f_i(x,y,0) = A_1 exp(-D(x+2)^2 - D(y+2)^2) \tag{43}$$

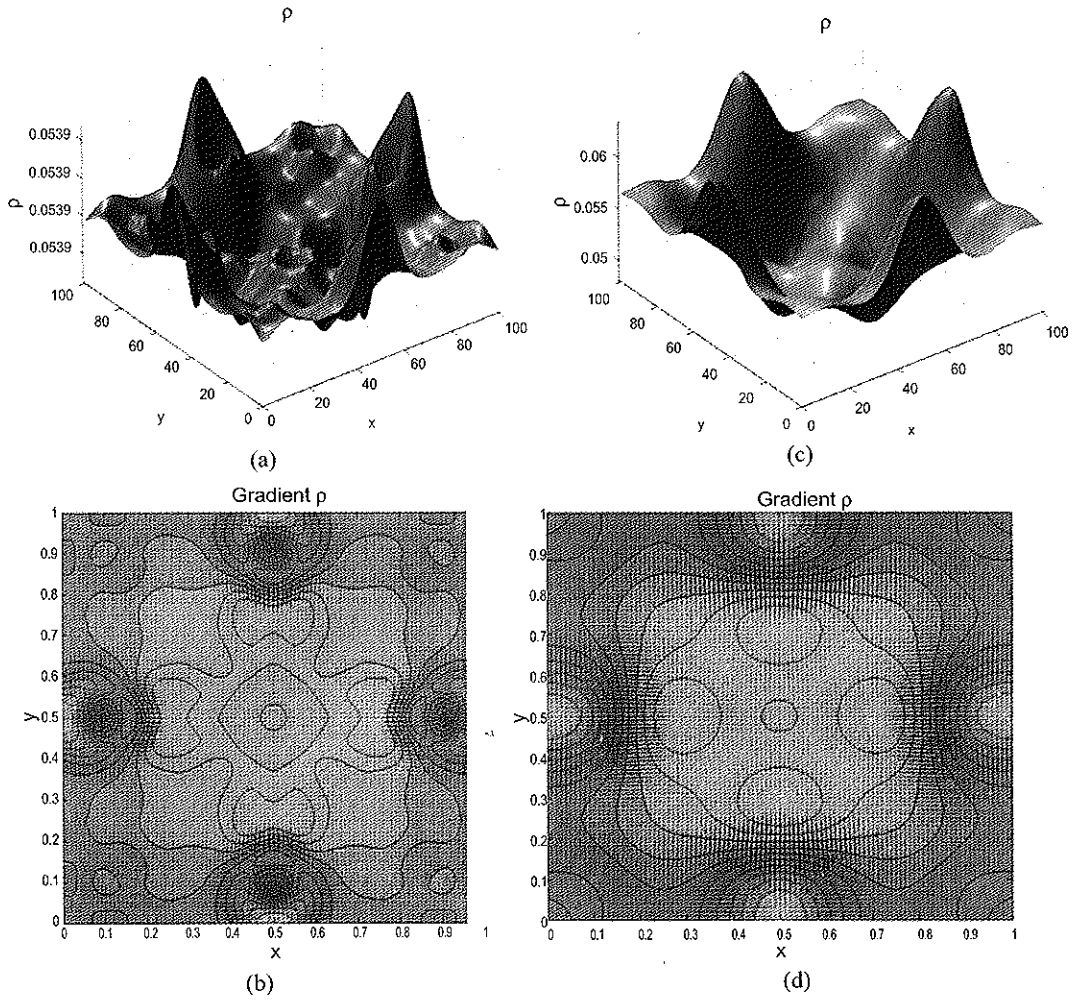

Fig.2. The numerical result of the d1q3 lattice Boltzmann model. Panels (a)-(d) correspond to simulations at times t = 140Δt. Parameters are: lattice size L = 100, κ =20,07, Δx = Δy = 1/L.

Then the algorithm initiates at $t_0 = 0$, with Eq. (42) or (43) in all the nodes of system. We present results for simulations in Figure (2), panels (a-d) for a system size of ***100x100***, with periodic boundaries conditions. In Figures (2) a-b, we show results for an initial Sine pulse and its gradient field. For Figures (2) c-d, we have the potential and the gradient field, respectively, for an initial Gaussian pulse.

5. Conclusions

We have solved the Poisson-Boltzmann equation using the lattice-Boltzmann technique. We obtain the structure of the potential and its gradient field for Sine and Gaussian initial configurations. This method can be easily extended to three dimensions. For a future paper, we can extend the method to explore phenomenology for unbalanced charge distributions.

7. Acknowledgments

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